An experimentally-validated multi-scale materials, process and device modelling & design platform enabling non-expert access to open innovation in the Organic and Large Area Electronics Industry (MUSICODE)

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Continuum modelling of solution processing by continuum mechanics

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Publishable summary

For the production of organic photovoltaic cells, the cost-effective wet process is used for mass production. In this process conjugated polymers and functionalized molecules are applied to a substrate together with a solvent as a liquid phase. The liquid layer is applied using an application system known as slot-die. The essential component of this system is a flat nozzle, which has approximately the width of the substrate and a defined distance from the substrate. The flow behavior of the dispersion can be influenced by optional heating in the slot die (hot end). The layer thickness of the liquid can be controlled by the applied mass flow, the nozzle spacing and the rotational speed of the cylinder in the R2R process or the belt speed in a flat system.

The formation of a defined structure from the liquid film takes place in a conditioning chamber. A key feature of this conditioning chamber is the heating of the substrate, which leads to a slowly evaporation of the solvent. Air or nitrogen flows through the conditioning chamber are used to remove the evaporated solvent. Due to the evaporation of the solvent, the polymers separate, and a bi-continuous structure is created, which thickness has only a fraction of the thickness of the original liquid film.

Computational fluid dynamics (CFD) is an established method to compute in a two or three-dimensional domain the flow field. The numerical solution of the Navier-Stokes equations is based on the discretization of the conservation equations. A common discretization scheme is the finite volume method. The simulation domain is therefore discretized by finite volumes. The discretized conservation equations are partial differential equations which are nonlinear. Fluid mechanics is a subfield of continuum mechanics.

To be able to predict the above-mentioned production process different physics have to be addressed. First, predicting the wet coating process the volume of fluid approach is needed which enables the simulation of a phase interface between gas and liquid and represents therefore a 2-phase simulation method. For the drying process in the conditioning chamber a film-model has been developed which interacts with the gas flow which is being numerically solved using the discretized Navier-Stokes-equation. To solve for the thermodynamic mixing (thermal and gas components) process the energy and concentration equations with the integrated gas-law is needed. The film model itself delivers the evaporation rate and film thickness. The evaporated solvent is added as mass source to the gas flow. Phase separation is solved using the phase field approach of the partner KIT in another scale (µm) using the film conditions from the macro scale (m).

For the MUSICODE modelling platform for the coating and drying process enhanced CFD-models have been developed and tested within WP2. Realistic model dimensions and operation conditions specified by OET and AUTh have been used to set up two separate models addressing the slot-die and the dryer. To be able to use the results of the slot-die model it has been directly linked to the dryer model transferring the resulting film thickness and film conditions (temperature, concentration). Further scales to be addressed via transferring data, are from the dryer to the phase separation model (KIT) and from that scale to the molecular dynamics model (UoI) is to be addressed in the cross-scale workflow of the modeling platform.